

### REMARKS

Claims 1-18 and 25-72 are pending; claims 1-18 and 25-36 have been withdrawn.

Claims 37-72 are addressed here. The independent claims of that group are claims 37 and 55.

#### Rejections Under 35 U.S.C. § 112

In the action mailed January 17, 2007, claims 52, 53, 70 and 71 were rejected as indefinite for listing values of charge without a sign. Applicants have made minor changes to those claims which are not believed to affect the scope of the claims, and which do not require any additional searching by the Examiner. Applicants therefore request that the amendments be entered.

#### Rejections Under 35 U.S.C. § 103

The Office Action makes two different rejections under 35 U.S.C. § 103 – one involving a combination of three different references, and another involving a combination of four different references. This is the first time that either rejection has been made in this prosecution.

Claims 37-47, 49-65, and 67-72 were rejected as obvious over the Huheey “Inorganic Chemistry” textbook (“the Huheey textbook”), an article by Marchi et al. in the Journal of Physics (“the Marchi article”), and a slide from a Powerpoint presentation by Crawford (“the Crawford slide”). Claims 37 and 55 are the independent claims.

Claims 37 and 55 recite, respectively, a machine and a computer-readable medium. The machine and medium generally include structure holding instructions for performing molecular dynamics simulations. In general, the simulations add dummy atoms to the actual structure of a metal ion. As noted in the pending application, such as at pages 7-10, a single atom ion may be

more accurately simulated using a polyatomic representation (e.g., four atoms surrounding the actual atom) in the form of a virtual ion, rather than in a single atom form. In the polyatomic representation, the dummy atoms may mimic the vacant orbitals of the metal ion, and thereby produce a result that might otherwise not be obtained using other forms of molecular dynamics simulations.

The Office Action suggests that the claims would be obvious because the Huheey textbook discusses crystal field theory (e.g., page 292, Figure 11.6 on page 397, and Table 11.6 on page 406, and Figure 11.15 on page 410) and also discusses ligands that, according to the Office Action, fit the criteria for “dummy atoms.” The Action states that the pending application defines “dummy atom” as “an atom that is assigned a van der Waals size of zero. That is, a dummy atom is basically a point charge.” The Office Action asserts that the Crawford slide discloses that crystal field theory “treats ligands as point negative charges.” The Action then asserts that the Marchi article discloses molecular dynamics simulations. The Office Action then suggests that a skilled artisan would have stitched together all of these disparate teachings – scattered across various portions of Huheey, and across the other two references, to have obviously produced the inventions recited in the pending claims.

Applicant respectfully disagrees, and notes that the application of the references here is plainly driven by impermissible hindsight. In particular, Huheey shows nothing more than general structures for actual ions. The fact that some of the ligands may be treated as point charges does not make them “dummy atoms” as recited in the pending claims. Rather, dummy atoms *are atoms added to the actual molecule and that that are assigned* a van der Walls size of zero, and are thus basically point charges. These are characteristics of dummy atoms, as recited

in the specification, but they are not a complete definition of “dummy atom.” Rather, by its very terms, a dummy atom is a made up atom—a “dummy” atom—that is added to a model to help in simulating a real world structure that does not include such an atom. As the pending patent specification explicitly notes, a dummy atom is “assigned” a certain size, thus confirming that it is an atom added for simulation, as discussed above.

The Office Action goes astray by improperly assuming that any point charge is a dummy atom, but that is a plain misreading of the passages the Office Action quotes out of the pending application. Those passages simply indicate that a van der Waals size of zero is a feature of the discussed dummy atom, but do not define “dummy atom” equal all atoms with a zero radius. Also, the passage cited by the Office Action notes that the radius is “assigned” to the dummy atom, thus further confirming that a dummy atom is an atom created for purposes of simulation. In addition, the passage from which the quote is lifted plainly speaks of molecular modeling, with the assignment of various charges and radii to atoms. Other portions indicate that a dummy atom “represent[s]” a vacant orbital. *See* Application, page 2, line 6.

With the claims viewed properly, it is plain that none of the prior art discusses anything about assigning particular values to atoms, such as by assigning a zero van der Waals radius so as to make a dummy atom. Rather, Huheey and the Crawford slide have nothing to do with simulation at all. And the Marchi article is wholly inapplicable because, to the extent it mentions simulations at all, it does so with respect to an alkalai ion surrounded by ammonia ions. There is absolutely nothing that would lead a skilled artisan to make up certain atoms known as dummy atoms, to which a van der Waals radius is assigned, so as to produce dummy atoms for a

simulation. The combination of these references is, in short, pure opportunistic hindsight that uses Applicants' invention as a template.

Claims 37, 48, 55, and 66 are rejected as obvious over the three references just discussed, in addition to an article by Maggiora in the "Journal of the American Chemical Society." Applicant respectfully requests that these rejections also be withdrawn in light of the discussion above regarding the pending independent claims. The addition of Maggiora does nothing to overcome the defects in the other references and in the arbitrary, hindsight-based combination of those references. Applicant thus respectfully requests allowance of all pending claims.

#### **Withdrawal of Finality of the Rejections**

Applicant respectfully submits that the finality of the present rejection is legally improper, and respectfully requests that it be withdrawn. Specifically, MPEP 706.07(a) makes plain that a final rejection is improper if the prior amendment should reasonably have been expected to have been claimed by the applicant:

"A second or any subsequent action on the merits in any application or patent involved in reexamination proceedings should not be made final if it includes a rejection, on prior art not of record, of any claim amended to include limitations which should reasonably have been expected to be claimed. See MPEP § 904 et seq. For example, one would reasonably expect that a rejection under 35 U.S.C. 112 for the reason of incompleteness would be replied to by an amendment supplying the omitted element."

In addition, MPEP 706.07 notes that prior art references should be applied in the first Office Action, and not held back:

Before final rejection is in order a clear issue should be developed between the examiner and applicant. To bring the prosecution to as speedy conclusion as possible and at the same time to deal justly by both the applicant and the public,

*the invention as disclosed and claimed should be thoroughly searched in the first action and the references fully applied;* and in reply to this action the applicant should amend with a view to avoiding all the grounds of rejection and objection.

That is precisely the case here. The prior Office Action rejected the claims under Section 112 and suggested that they be amended to monoatomic ions for reasons of enablement; Applicant complied. The prior Office Action made no prior art rejections, and thus denied Applicant the opportunity to address such rejections, even though they could have been made at the time. Applicants' amendments—to add “monoatomic”—would not have required any additional searching, and were in fact the amendments called out and suggested by the Office Action. As a result, Applicant has been denied a right to develop a clear issue with respect to the prior art, which could have been and should have been applied in the prior Office Action. Applicant thus respectfully requests that the finality of the rejection be withdrawn, if the claims are not allowed.

It is believed that all of the pending claims have been addressed. However, the absence of a reply to a specific rejection, issue, or comment does not signify agreement with or concession of that rejection, issue, or comment. In addition, because the arguments made above may not be exhaustive, there may be reasons for patentability of any or all pending claims (or other claims) that have not been expressed. Finally, nothing in this paper should be construed as an intent to concede any issue with regard to any claim, except as specifically stated in this paper, and the amendment of any claim does not necessarily signify concession of unpatentability of the claim prior to its amendment.

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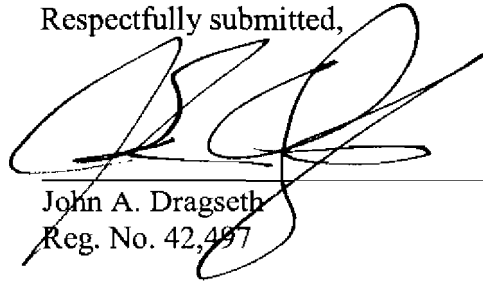
Applicant : Yuan-Ping Pang  
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Respectfully submitted,

Date: \_\_\_\_\_

3/19/07

A handwritten signature in black ink, appearing to read 'J. Dragseth', written over a horizontal line.

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